CONTROLLING PHOTONS AND CHARGE CARRIERS INTERACTIONS IN GRAPHENE SHEETS WITH HALIDE PEROVSKITE LAYERS

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ABSTRACT. In the pursuit of highly efficient photovoltaic absorbers, halide perovskites are real prospects, but they lack stability and recombinations limit their efficiency. To fix current shortcomings, I propose to widen the range of investigations. In particular, I am seeking to advance the optoelectronic properties of graphene sheets with metal halide perovskite layers. Lowering recombination rates is a challenge for perovskites that may be addressed by transferring charge carriers from the perovskite to the graphene layers. Various synthetic strategies would be methodically elucidated in the aim of enhancing the efficiency of both perovskite solar cells, transistors and light emitters. This proposal may have remarkable outcomes for energy efficient technologies.

BACKGROUND

In the past five years, metal halide perovskites have drawn huge excitement from the photovoltaics research community because of their high power conversion efficiency. The 2D-structured perovskite demonstrate promising stability properties[1], large carrier mobility[2], strong light absorption, superb photo- and electro-luminescence[3,4] and strong quantum confinement effects. These properties have enabled LEDs[5,6], lasers and photodetectors[7] powered with perovskite materials.

In the realm of 2D materials, the use of stacked layers, forming so-called van der Waals heterostructures, has empowered in-band structure engineering[8] to create tunnel junctions with unparalleled performances. To date, the best materials for building such heterostructures have been graphene, frequently achieving superior performances for surface science, endowing it with favourable electronic, optical, thermal and mechanical properties[9].

This proposal aims to create heterostructures based on graphene sheets with layered 2D perovskites. This challenge has been addressed with thin film perovskites and has shown excellent FET performance but poor stability in ambient conditions[10]. Here, two dimensional perovskite may be a promising alternative for enhanced stability and attractive electronic and optical properties[11]. Moreover, 2D perovskite can be bound to graphene sheets by various techniques as I present in this research proposal.

PROJECT DETAILS

Scope of the project I propose to investigate various bonding strategies between 2D perovskite layers and graphene sheets to create stacks and assess their properties. Various synthetic methods as well various bond types may be explored: van der Waals, ionic, covalent and hydrogen bonds[12].

The question to be addressed is: to what extend does the nature of the bonding between graphene sheets and 2D perovskite layers influence the optoelectronic properties of the stack?

Approaches Graphene and perovskite space groups are different

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therefore stacking the two materials in a heterostructure will induce lattice strain. However, interface modelling studies[13] showed that this kind of heterostructure can be stable.

Van der Waals heterostructures will be manufactured via physical deposition under vacuum. Ionic heterostructures will be developed by doping the graphene structure to make it more or less electroattractive. Hydrogen and covalent bonding will involve structure modification, enabled by the 2D perovskite where the crystallographic structure is not influenced by the cation[14]. Thus both the excitonic energy and the bandgap will stay unchanged. However, it may require the modification of graphene via grafting organic cations molecules on its surface.

Van der Waals heterostructures of graphene and perovskite have been theorised[13]. It has been predicted that the electronic structure of both 2D halide perovskite and graphene will be preserved after stacking. To my knowledge, there has never been any attempt to carry out the practical experiment.

With grafting methods, I anticipate that recombination rates may be reduced by transferring charge carriers from the perovskite to the graphene layers. This may lead to higher efficiency solar cells. Finally, I anticipate that the different binding approaches will tune the position of the Fermi level by modifying the interface between the two layers. The orbital overlapping may be altered, as well as the electronic configuration at the interface.

Methodology The sample preparation would be carried out in the stimulating environment of the Condensed Matter Physics Group at the University of Manchester.

Characterisation of the manufactured materials would be carried out with X-Ray Diffraction techniques, as well as observations with Scanning and Transmission Electron Microscopy. The optoelectronic properties would be explored via photoluminescence spectroscopy; charge transport with microwave conductivity measurements; surface states with transient absorption spectroscopy; and the band structure with Compton and Raman scattering.

Timeline The first year of the PhD would be dedicated to exploring the property range through methodical testing, with the aim of identifying the most efficient process for keeping the heterojunction stable. During the two following years, I would focus on the optoelectronic properties of the manufactured materials. The various bonding investigations would be carried out simultaneously in order to be able to compare results.

OBJECTIVES AND FINAL OUTCOMES

I believe that combining two outstanding materials may lead to unparalleled results. Covalent bonding will affect the graphene conjugation system, therefore compromising some of its properties. I suppose that non-covalent interactions may preserve all of its electronic properties. The afforded assembly with two-dimensional perovskite structures may certainly give rise to a new class of layered semiconductors, as the assembly with the bulk perovskite counterparts already gave astonishing performances[10].

I am convinced that both graphene and perovskite are classes of materials that have the potential to impact the future of modern civilisation. My investigations may lead to meaningful industrial opportunities with great impact on energy saving and energy collection.

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